Nonsymmorphic topological semimetals and interaction driven topological phases

Chen Fang
Institute of Physics
Chinese Academy of Sciences

Acknowledgements

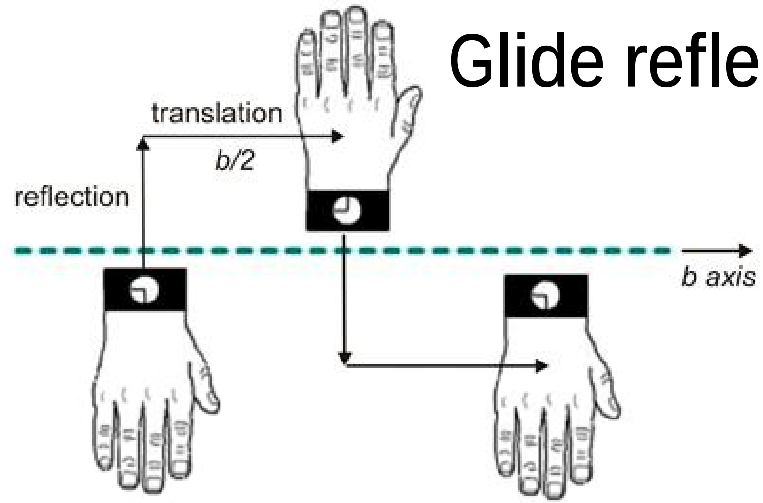
- MIT
  - Junwei Liu
  - Liang Fu
- IOP
  - Zi Yang Meng
  - Ling Lu
- Renmin University
  - Han-Qing Wu (now at UC at Northbridge)
  - Yuan-Yao He
  - Zhong-Yi Lu

Outline

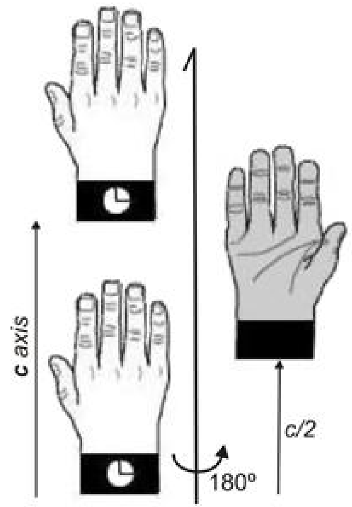
- Nonsymmorphic topological semimetals
  - Helicoid surface states of a Weyl semimetal
  - Double-helicoid surface states of a nonsymmorphic Dirac semimetal
  - Tetra-helicoid surface states
- QAH driven by weak repulsion
  - Quadratic band touching on a checkerboard
  - Chern number and rotation eigenvalues
  - Diagnosis using exact diagonalization

Nonsymmorphic symmetries

- A nonsymmorphic symmetry operation is the composition of a point group operation and a fractional lattice translation.
- Glide reflection = mirror reflection + in-plane half-translation
- Screw rotation = rotation + half-translation along axis

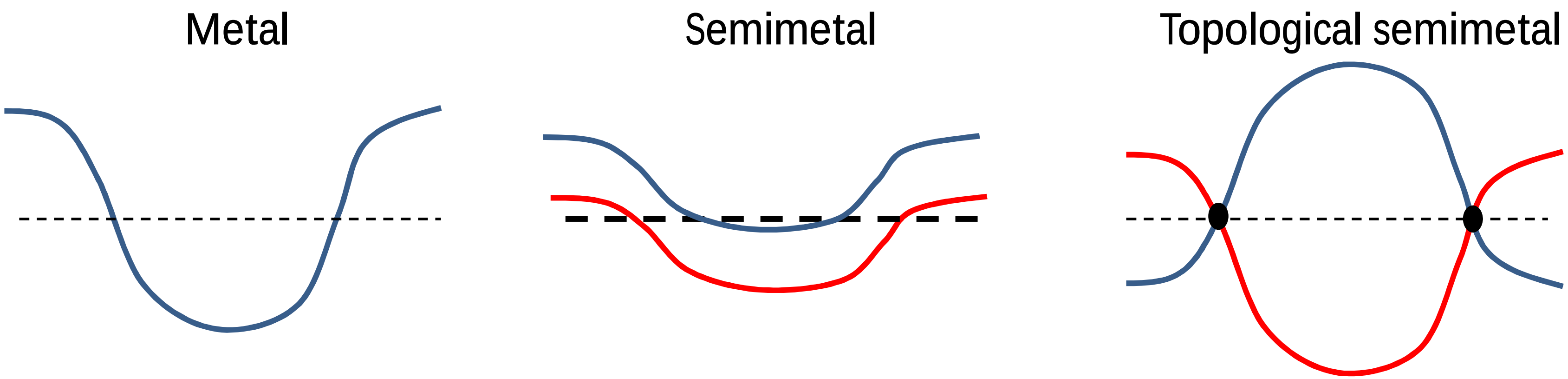


Glide reflection



Screw rotation

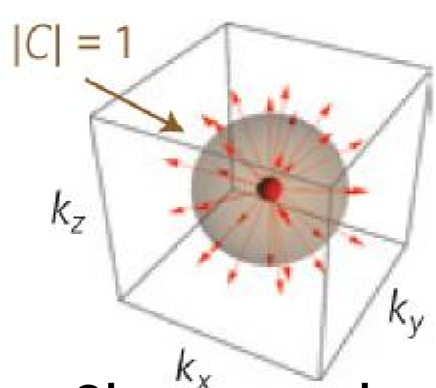
Topological semimetals



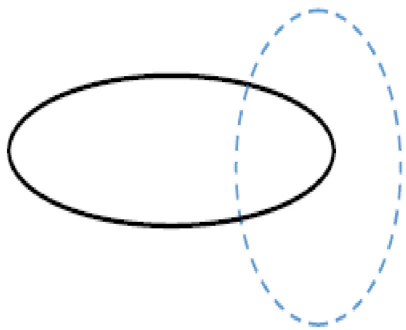
- Topological semimetals have the conduction and the valence bands crossing each other, and the crossings cannot be removed by perturbations preserving certain symmetries.
- At generic filling, the Fermi surface of a TSM has nontrivial topological number(s).

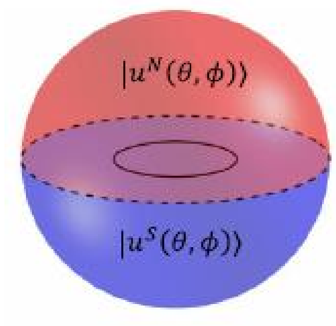
Topological gapless band structure

- Enclose the band crossing with a surface in k-space, such that on the surface the bands are separated and the topological invariants are defined on the enclosing surface.
- It can also be considered as the topology of the Fermi surface at a generic filling.



Chern number

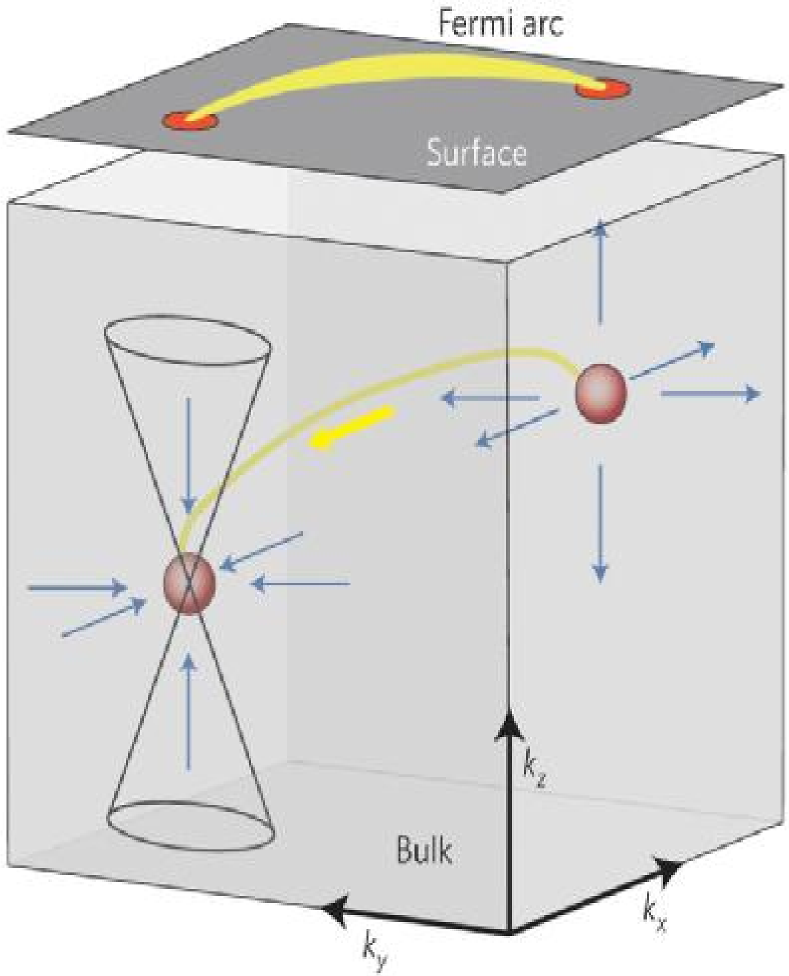

Berry phase



New Z_2 charge

Weyl semimetals

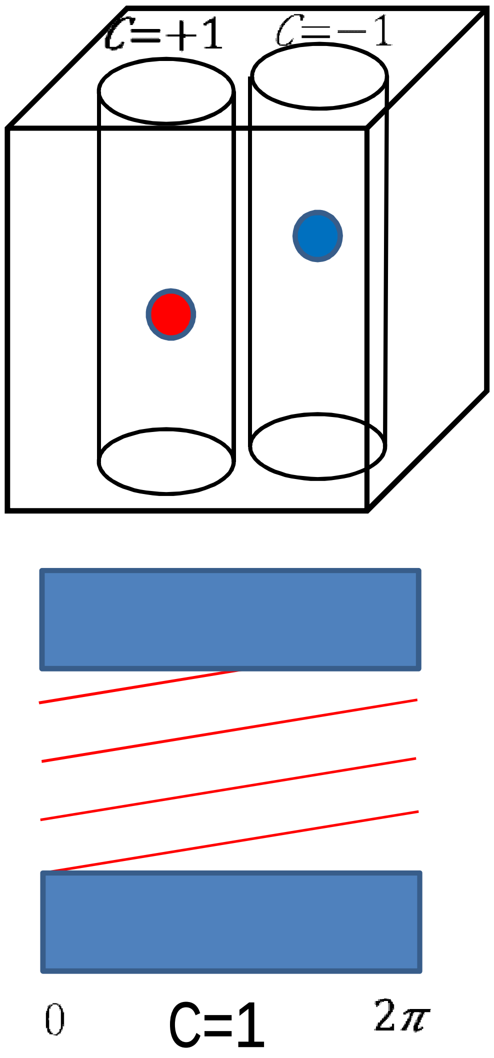
- Breaking at least one of time-reversal and inversion
  - If T-breaking, 2n Weyl points
  - If P-breaking, 4n Weyl points
- Each Weyl node has either +1 or -1 monopole charge
- Near Weyl point the effective theory is the Weyl equations
- A Fermi arc connects the projections of a pair of Weyl points on the surface



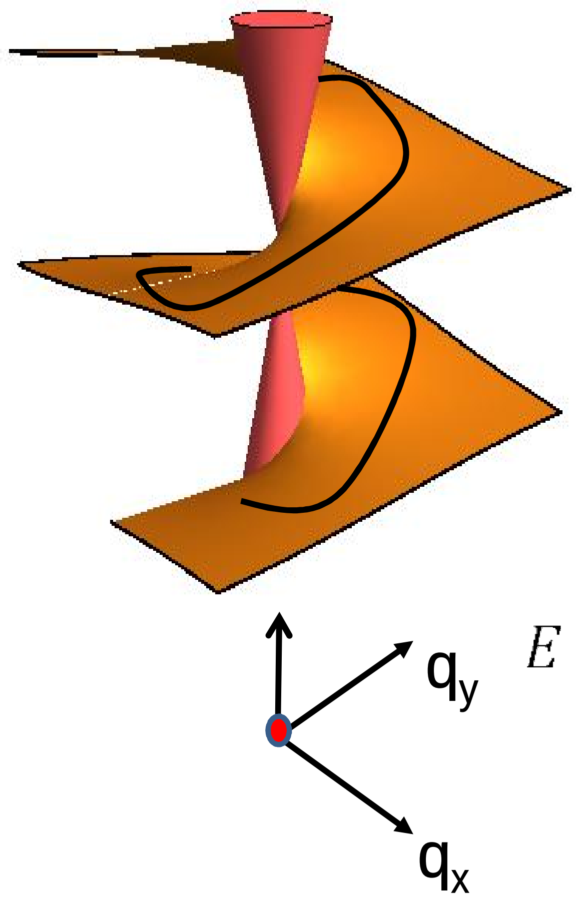
Bernevig, Nat. Phys. (2015)

CF*, L. Lu, J. Liu and L. Fu*, Nature Physics 12, 936 (2016)

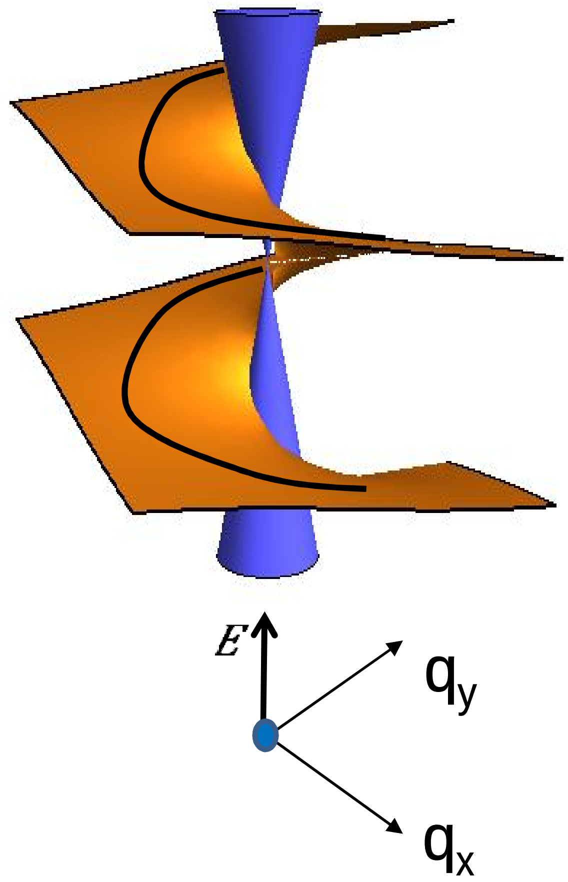
Helicoid surface state



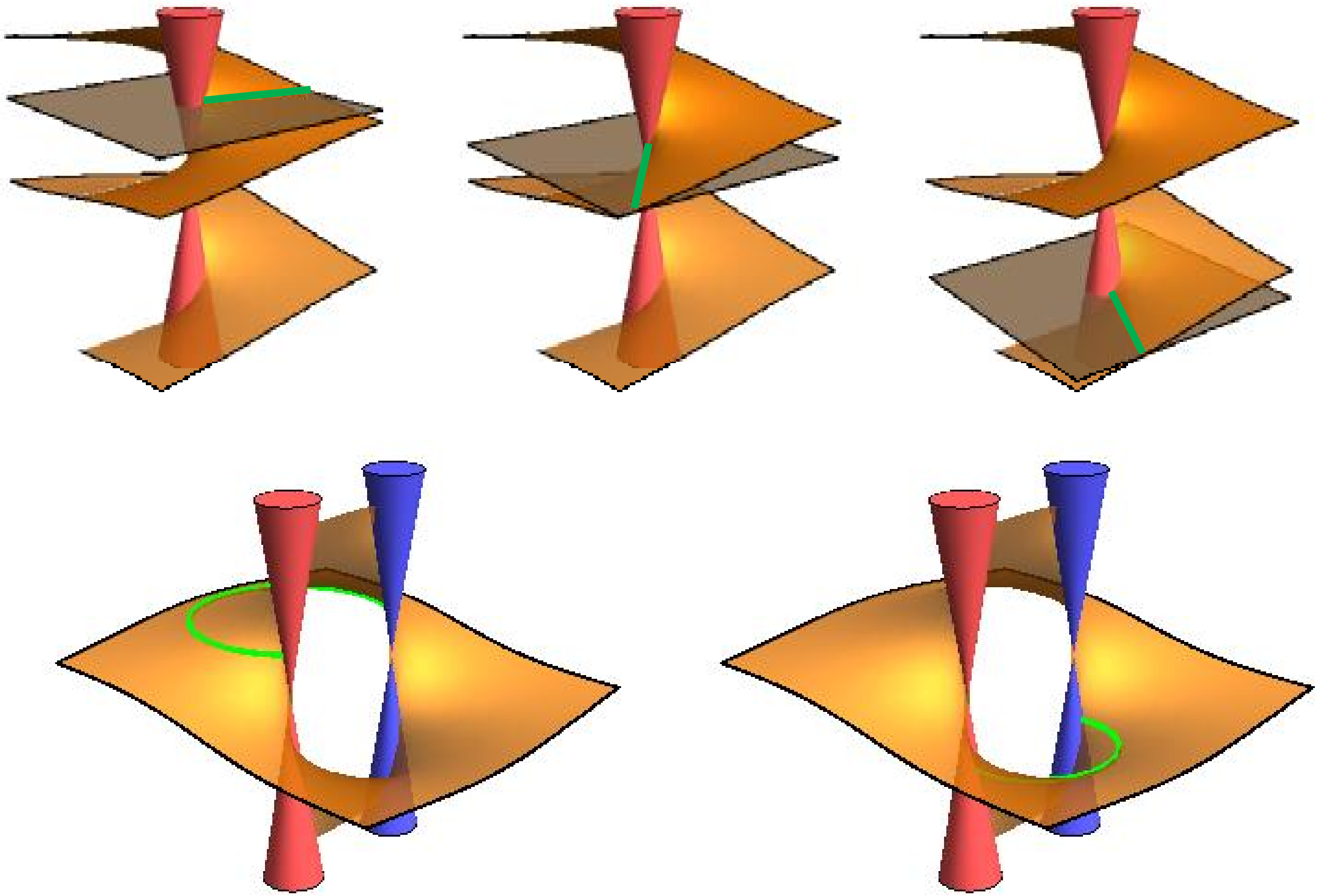
Positive Weyl



Negative Weyl



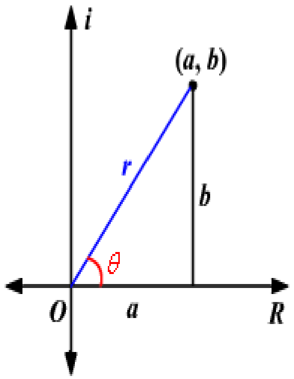
Fermi arcs

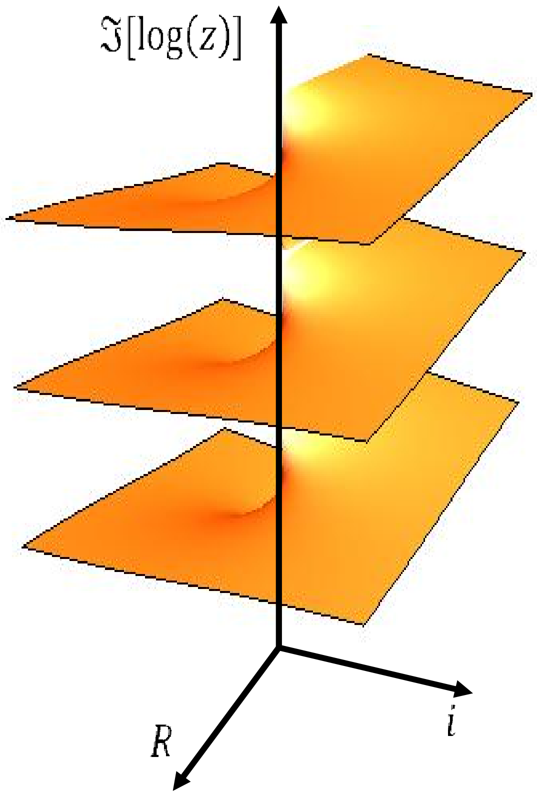


Riemann surface

- A Riemann surface is a surface-like configuration that covers the complex plane with several, and in general infinitely many, "sheets.“ (from Wolfram MathWorld)

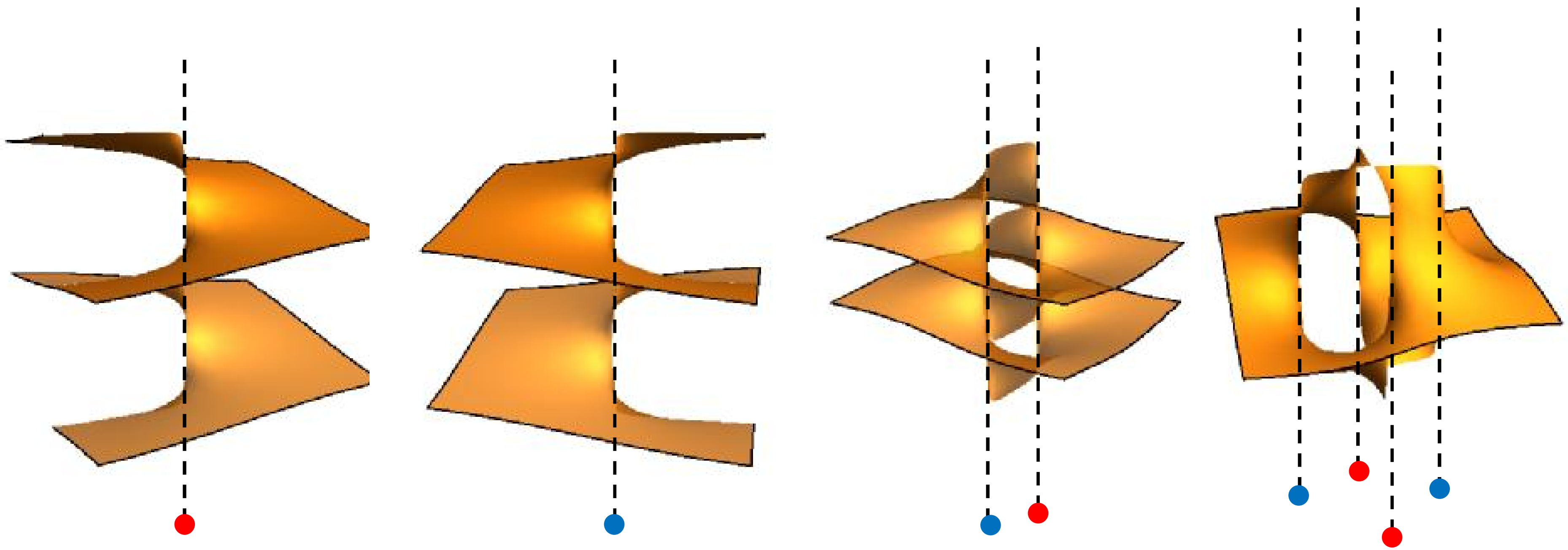
$\log(z) = \log(r) + i(\theta + 2n\pi),$
$n \in$ Ingeters





$$E(k_x, k_y) \sim \mathrm{Im}[\log(k)]$$
$$k = k_x + ik_y$$

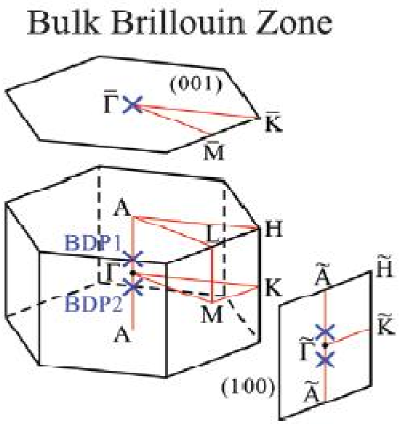
Riemann surfaces for Weyl semimetals



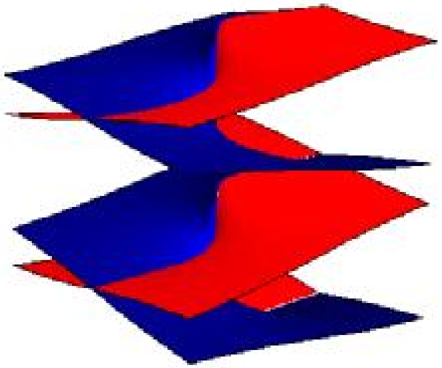
$\log(k)$ $\log(k^{-1})$ $\log(\frac{k-a}{k-b})$ $\log[\frac{(k-a)(k-c)}{(k-b)(k-d)}]$

Dirac semimetal

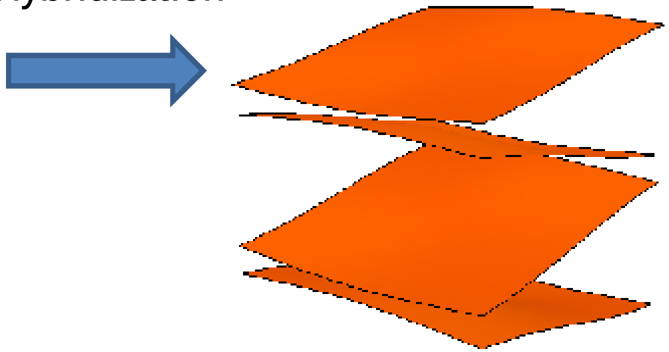
- A Dirac point can be considered as the superposition of two Weyl points with opposite Chern numbers at the same position in the momentum space.
- It takes additional symmetry (e.g., rotation) to prevent the annihilation of the Weyl points.
- On the surface, there are two counter-propagating spirals, but not stable against hybridization.



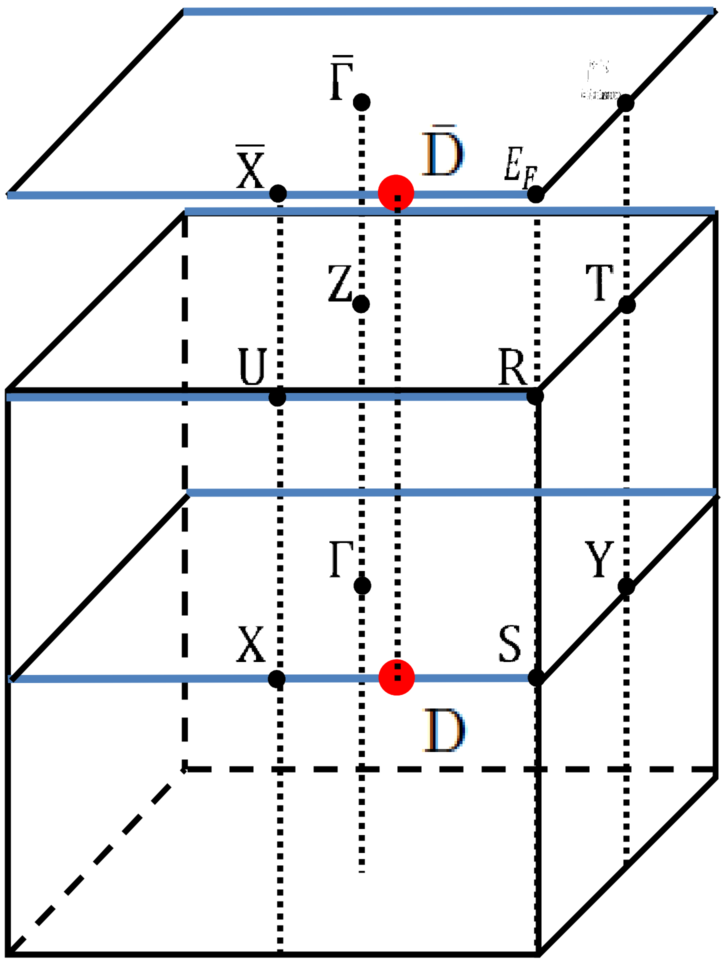
Na_3Bi



Hybridization



Kramers'-like line-degeneracy



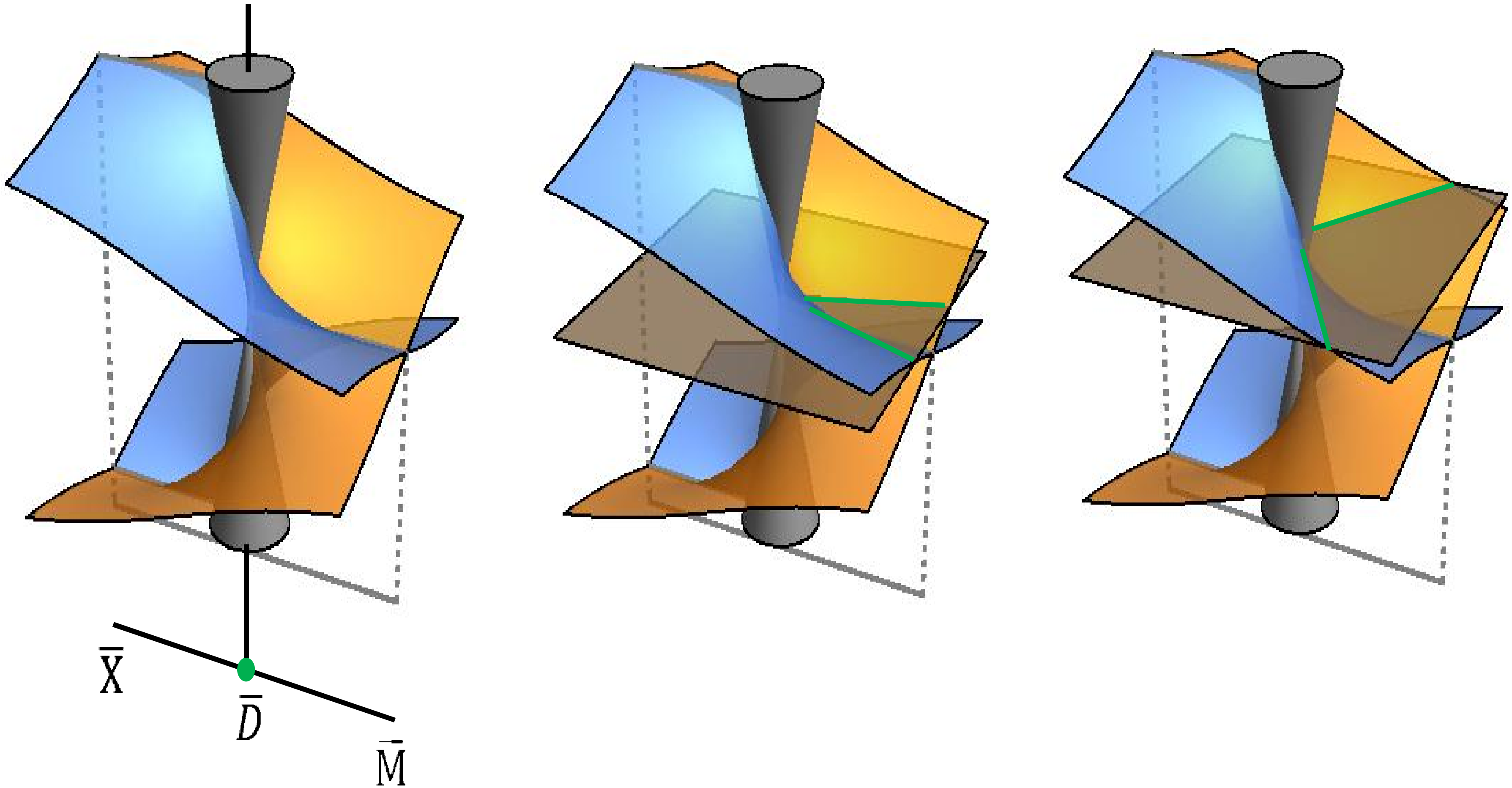
$$G : (x, y, z) \to (-x, y + 1/2, z)$$

$$(G * T)^2 = T_y = e^{-ik_y}$$

$$G * T : (k_x, k_y, k_z) \to (k_x, -k_y, -k_z)$$

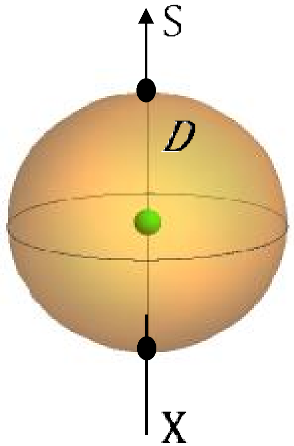
Double-helicoid Riemann surface states

$$E(k) \sim \mathrm{Im}[\log(k + k^{-1} + \sqrt{k^2 + k^{-2} - 2})]$$



Z_2 invariant in the bulk

- G*T ensures the existence of a smooth gauge on the sphere
- (G*T)^2=-1 at the BZ boundary allows to define the Pfaffians for the sewing matrix at two points on the sphere.
- A Fu-Kane-like formula in the presence of inversion

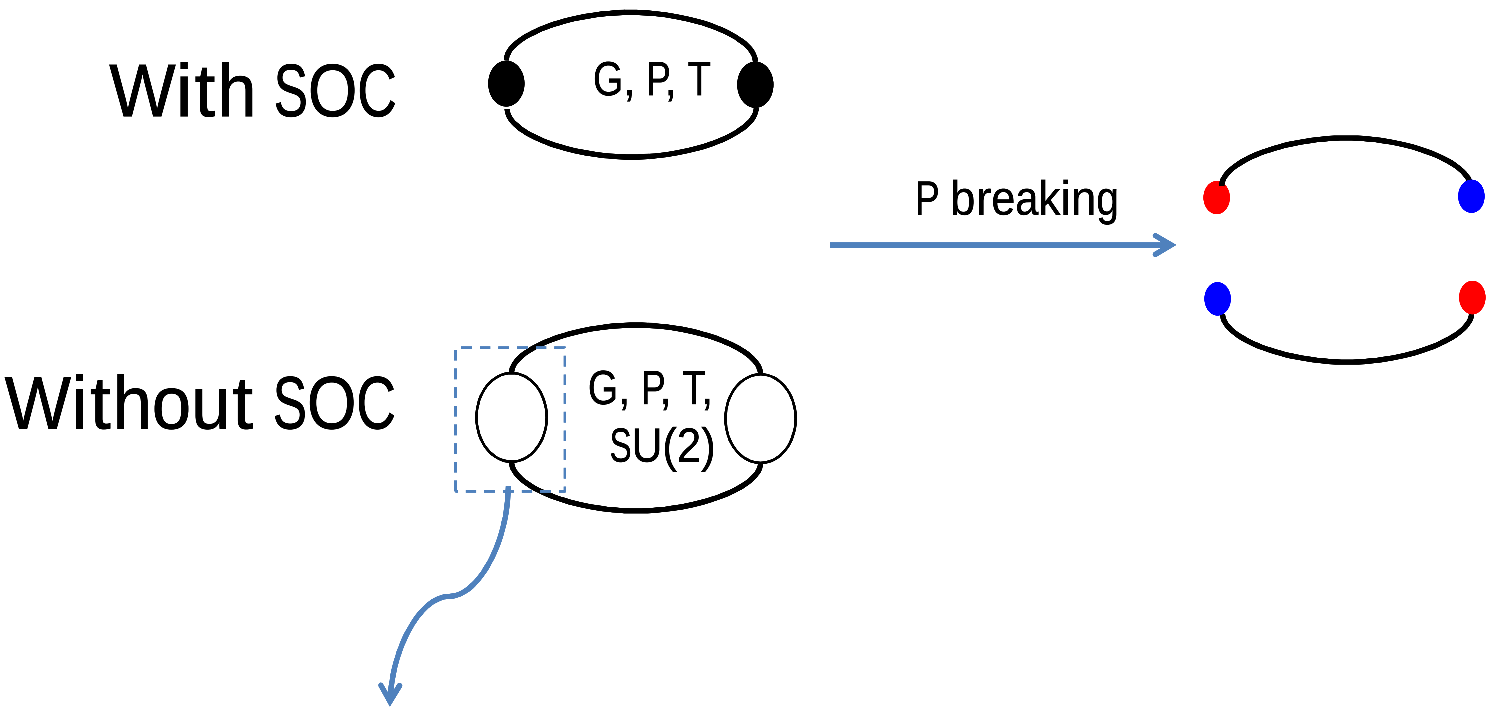


$$G * T: (\theta, \phi) \to (\theta, \phi + \pi)$$

$$W(\theta, \phi) \equiv \langle u_m(\theta, \phi + \pi) | G * T | u_n(\theta, \phi) \rangle$$

$$(-1)^{\delta} = \frac{\mathrm{Pf}[W(0)]}{\sqrt{\det[W(0)]}} \frac{\mathrm{Pf}[W(\pi)]}{\sqrt{\det[W(\pi)]}} \xrightarrow{P} \prod_{n \in occ./2} \frac{\gamma_{2n}(0)}{\gamma_{2n}(\pi)}$$

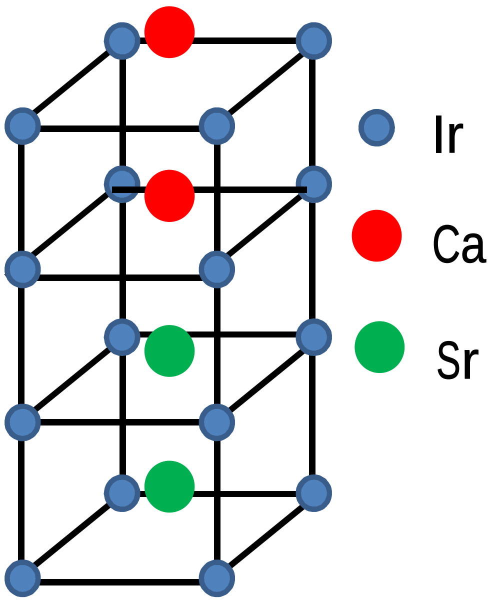
Breaking of nonsymmorphic Dirac point

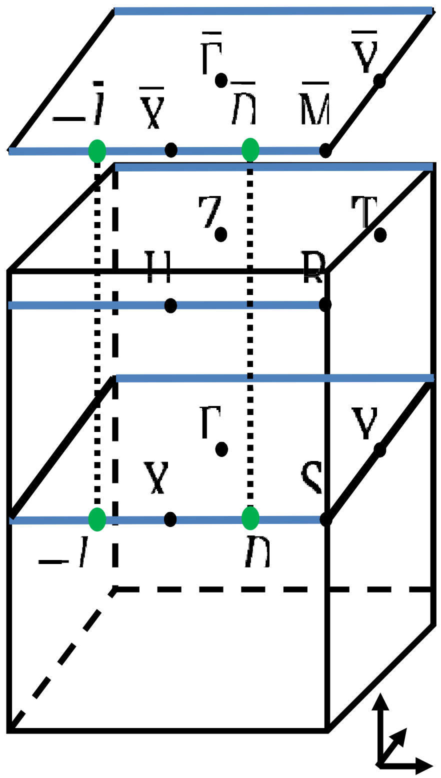


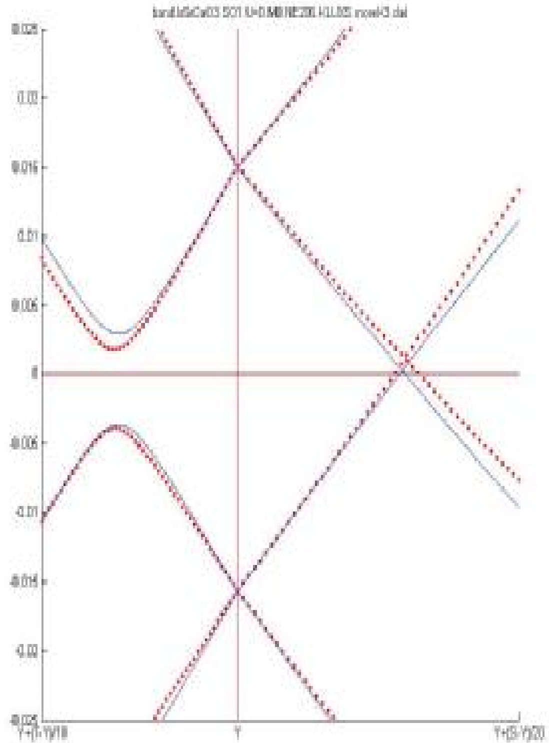
Nodal ring with surface arcs
Nodal ring with new Z_2

Nonsymmorphic Dirac point

$$G:(x,y,z)\rightarrow(-x,y+\frac{1}{2},z)$$

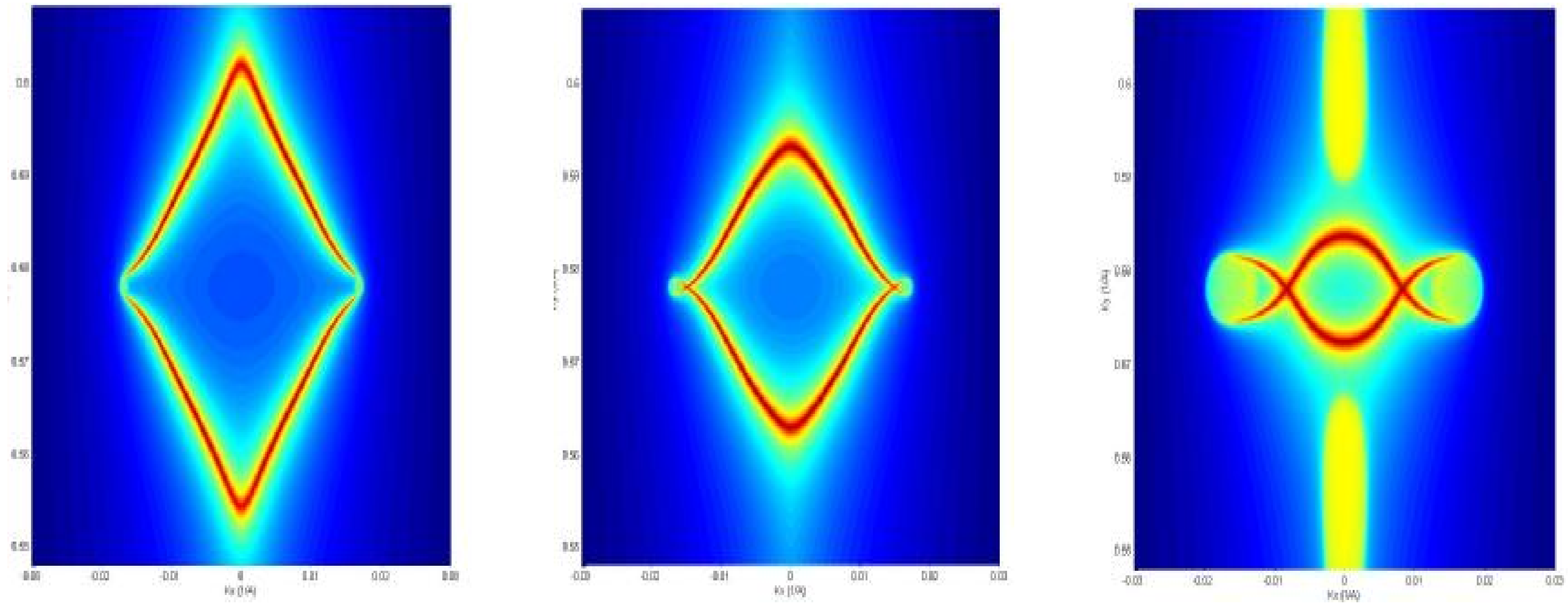






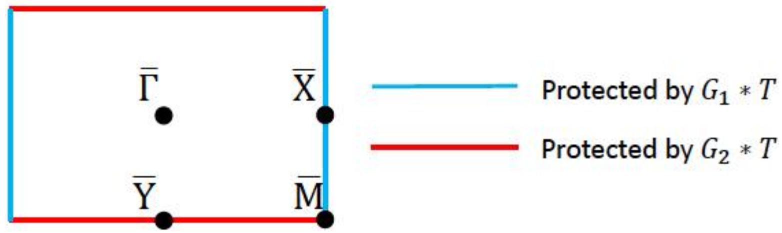
Protected by G*T

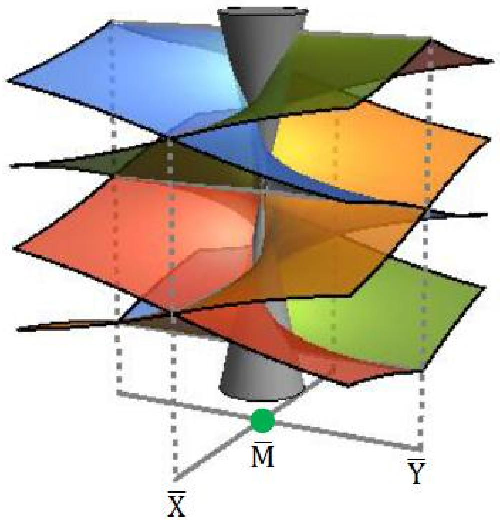
(001)-surface states of $(SrIrO_3)_2(CaIrO_3)_2$



Tetra-helicoid surface state

- Two glide planes and time-reversal ensures double degeneracy along two high-symmetry lines.
- A topological nontrivial dispersion can exist around M.
- No bulk invariant (conjecture).
- May be a filling enforced semimetal (conjecture).

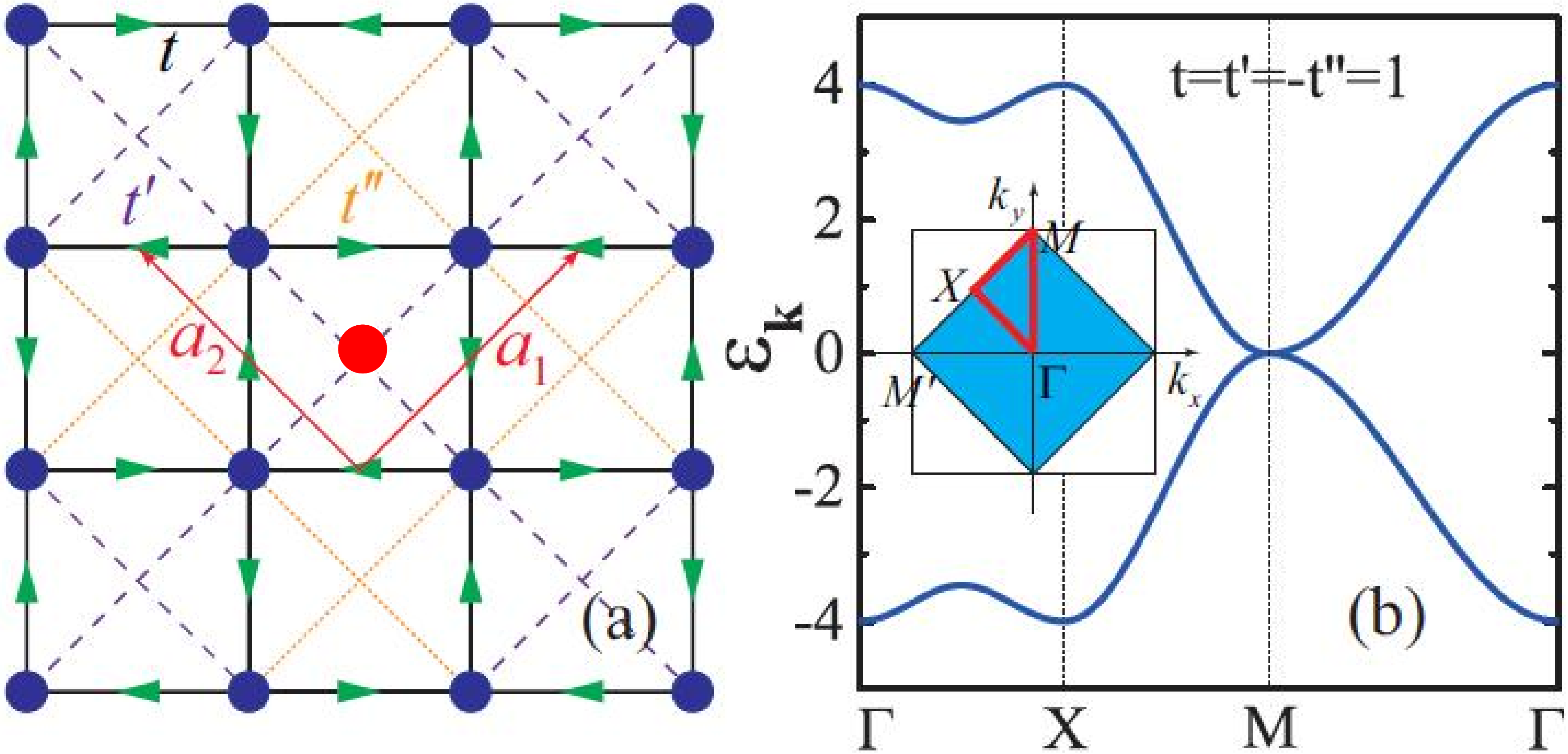




$$E(k) \sim \Im\left[\log\left(\sqrt{k^2 + k^{-2} + 2} + \sqrt{k^2 + k^{-2} - 2}\right)\right]$$
$$k = k_x + ik_y$$

K. Sun, H. Yao, E. Fradkin, and S. A. Kivelson, Phys. Rev. Lett. 103, 046811 (2009)

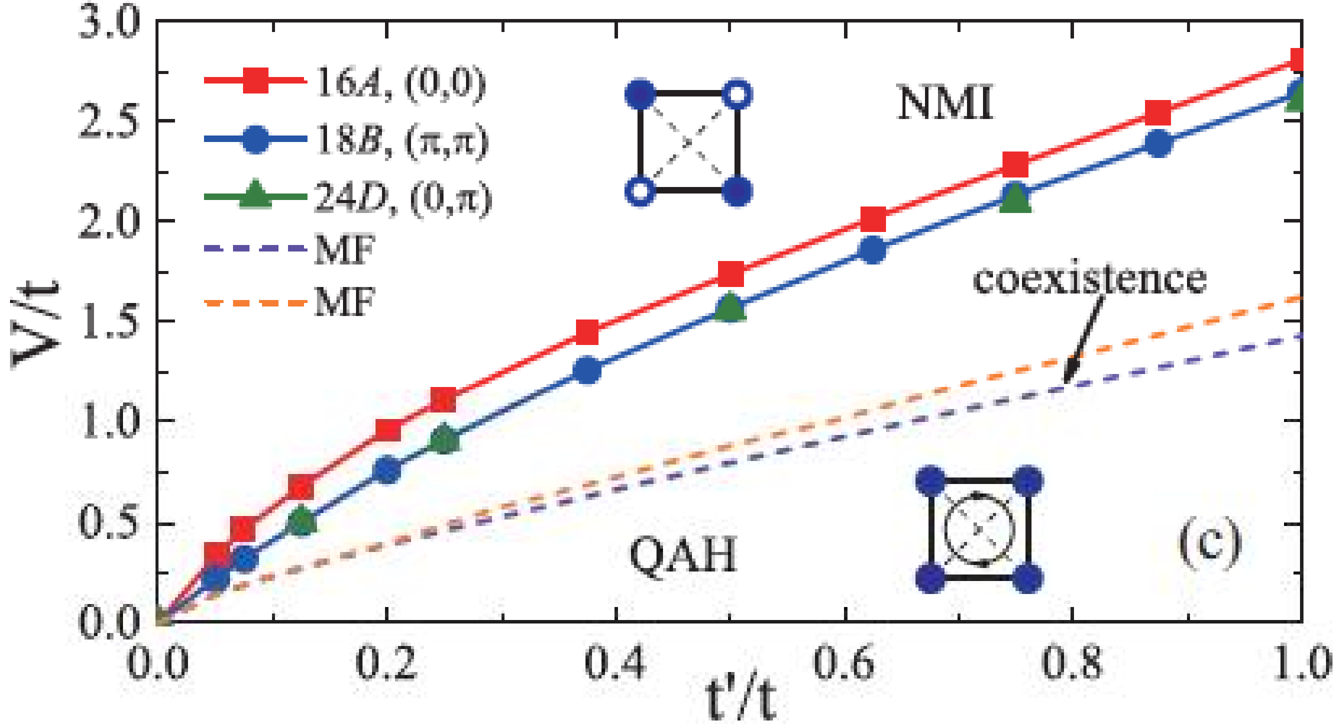
Quadratic band touching



- C_4-rotation eigenvalues are +i and –i at M, and time-reversal pins them together.
- The dispersion around M is quadratic in both directions and time-reversal ensures zero winding.

Mean field phase diagram

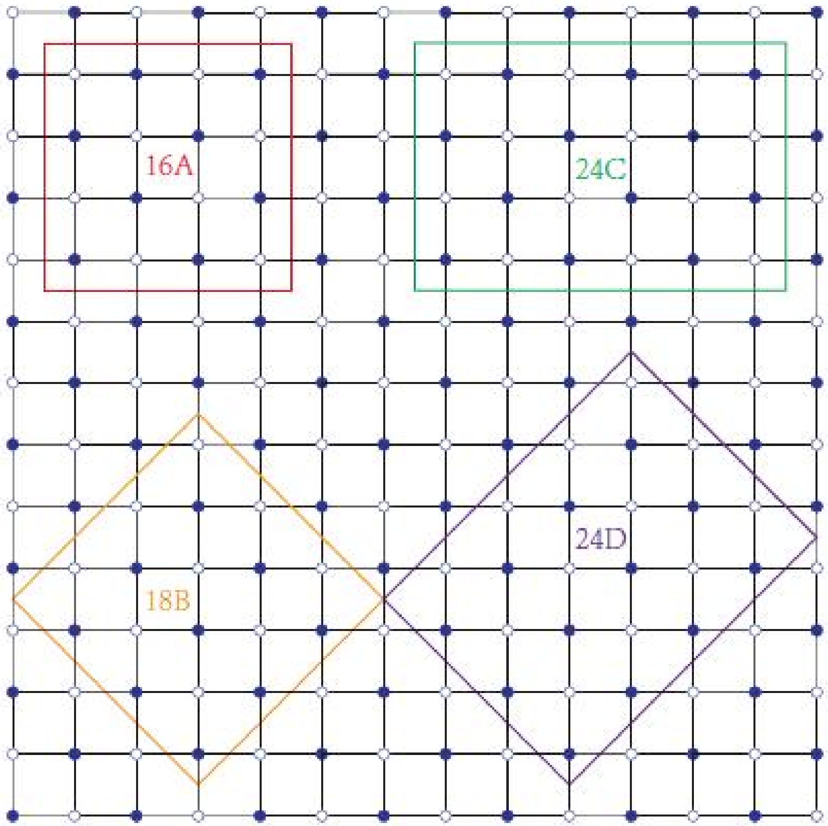
$t'/t''=-1$



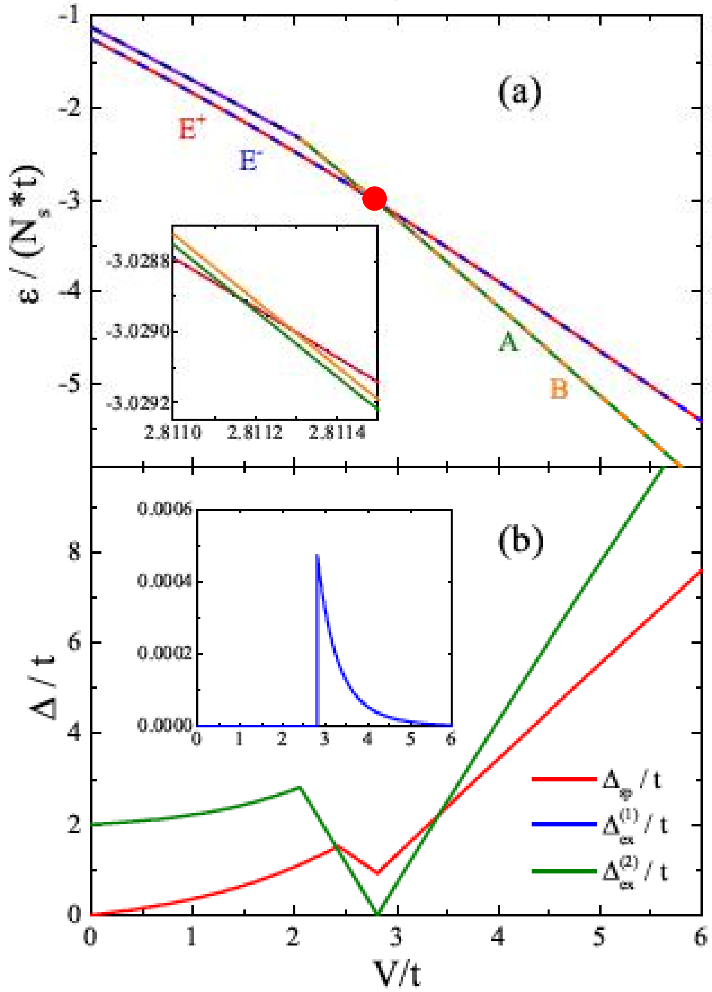
Phase	C_4	T	Chern
QAH	Yes	No	+-1
NMI	No	Yes	0

H.-Q. Wu, Y.-Y. He, CF*, Z. Y. Meng*, and Z.-Y. Lu, Phys. Rev. Lett. 117, 066403 (2016)

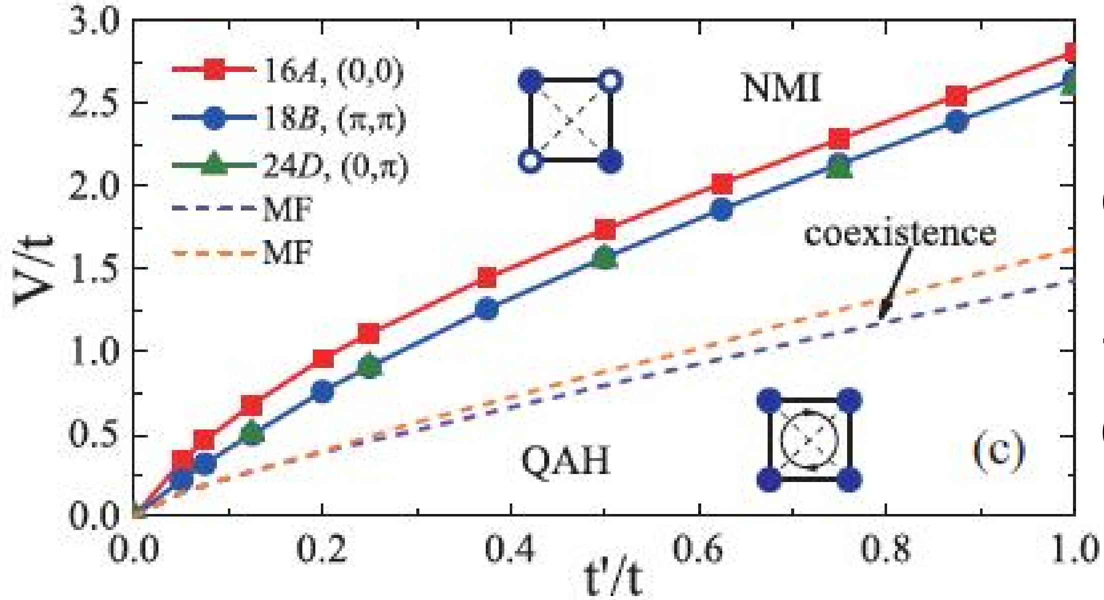
Exact diagonalization



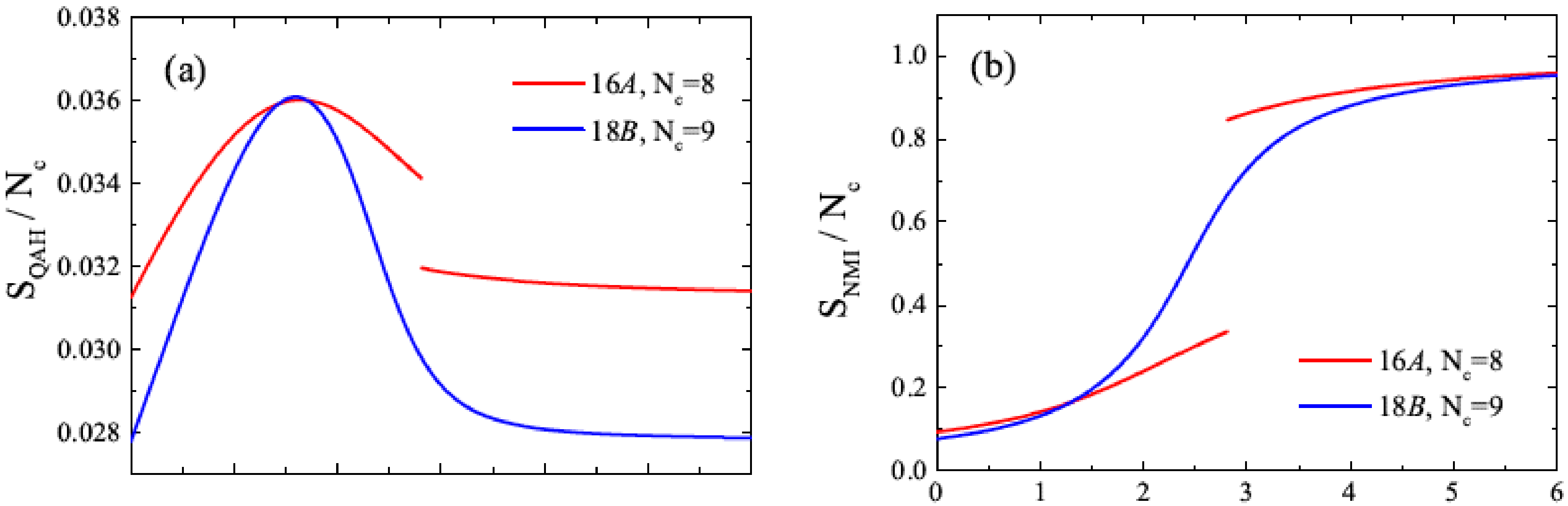
t/t′=1, t′/t′′=-1



Exact diagonalization

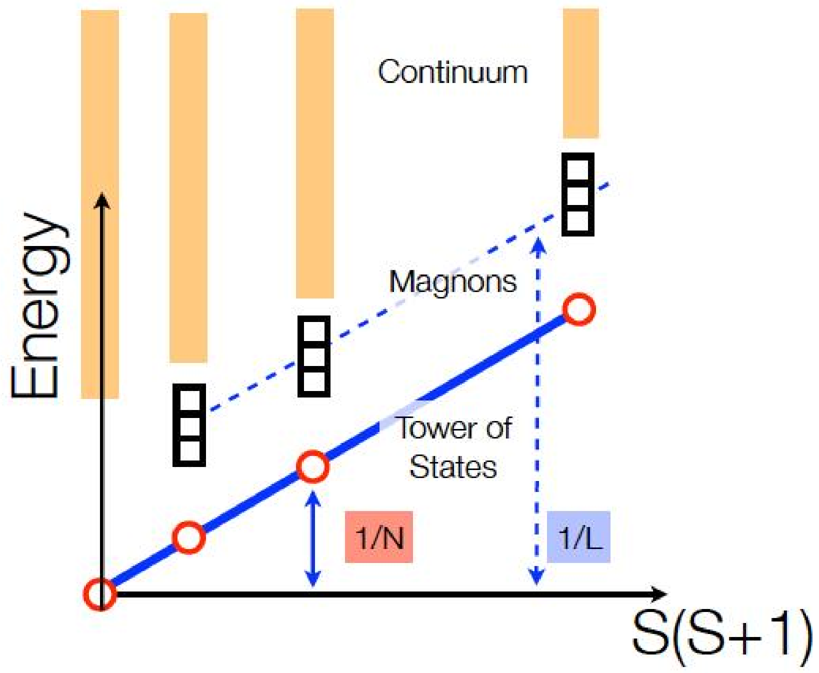


Results are suggestive of the two phases, but but QAH correlation is too weak to be conclusive.



Anderson’s tower of states

- Generically, the exact ground state has no symmetry breaking.
- The thermodynamic ground state comes from the superposition of exact eigenstates in the “tower of states”
- The “tower of states” are lower in energy than any elementary excitation, and represent a global motion.

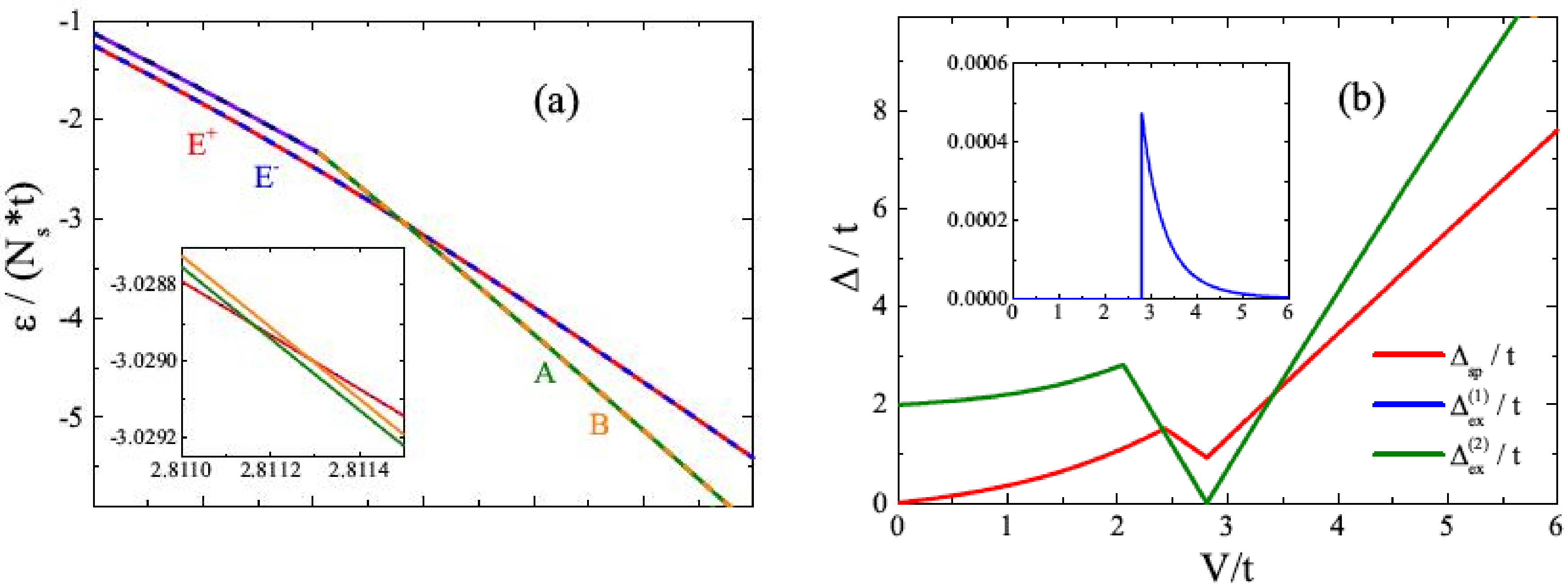


Change of C_4-eigenvalues

Blue=+i
Red=-i
Green=+1
Yellow=-1

Tower of states

$V<V_c$: Blue = Red < Green < Yellow
$V>V_c$: Green < Yellow < Blue = Red



CF, Matthew J. Gilbert, and B. Andrei Bernevig, Phys. Rev. B 86, 115112 (2012)

Chern number and rotation eigenvalues

- Chern number does not need any symmetry for protection, but symmetry can simplify its calculation.
  - No interaction:

$$i^C = \prod_{n\in occ} \xi_n(\Gamma)\xi_n(M)\zeta_n(X)$$

  - Arbitrary interaction:

$$i^C = \xi(0,0)\xi(\pi,\pi)\zeta(\pi,0)$$

  - Weak interaction (even-by-even lattice):

$$i^C = \xi(0,0)$$

Blue: C=+1, Red: C=-1, Green: C=0, Yellow: C=0

No superposition of states with different topological numbers

- The superposition is due to random local pinning field.
- Selection rule: the matrix element of any local operator between states with different Chern numbers must vanish, or one could change the topological number by using a local field.

$$H = J \begin{pmatrix} \langle \Omega | \hat{O} | \Omega \rangle & \langle \Omega | \hat{O} | \Omega' \rangle \\ \langle \Omega' | \hat{O} | \Omega \rangle & \langle \Omega' | \hat{O} | \Omega' \rangle \end{pmatrix}$$

Symmetry analysis

interaction	$\xi(0,0)$	SSB	Chern number
$V < V_c$	$\pm i$	TRS	± 1
$V > V_c$	± 1	$C_4 \to C_2$	0

- For $V<V_c$, since the two states have different Chern numbers, the GS cannot be a superposition, so it preserves C_4 but breaks TRS.
- For $V>V_c$, the two states have both zero Chern number, so the GS is generically a superposition and breaks C_4 down to C_2.

Conclusions

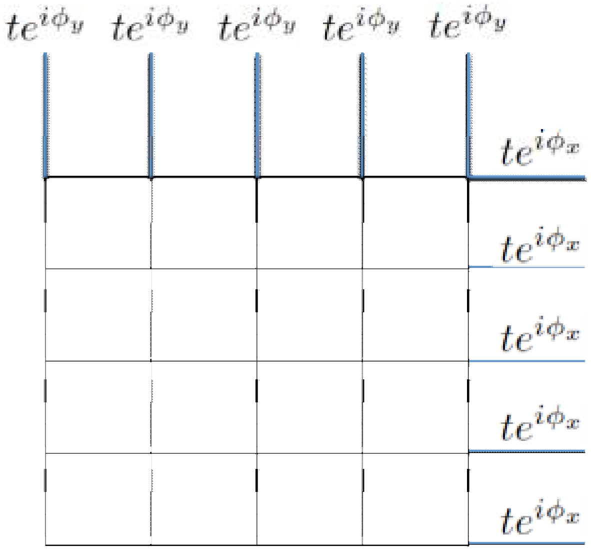
- Nonsymmorphic topological semimetals

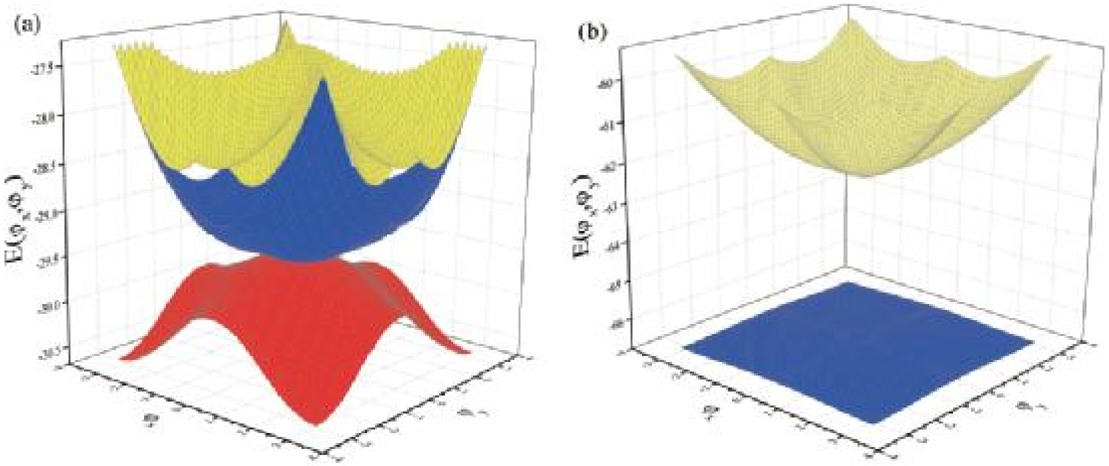
  CF*, L. Lu, J. Liu and L. Fu*, Nature Physics 12, 936 (2016)
  - Glide plane along with P and T can protect Dirac points at BZ boundary;
  - Such Dirac points have PROTECTED surface arcs;
  - Dispersions of WSM and nonsymmorphic DSM can be mapped to noncompact Riemann surfaces;
  - $(SrIrO_3)_2(CaIrO_3)_2$ is predicted to be nonsymmorphic DSM.
- Interaction driven topological phases

  H.-Q. Wu, Y.-Y. He, CF*, Z. Y. Meng*, and Z.-Y. Lu, Phys. Rev. Lett. 117, 066403 (2016)
  - Point group eigenvalues are related to the topological numbers (Chern numbers);
  - Thermodynamic ground state cannot be superposition of quantum states with different topological numbers;
  - Checkerboard lattice with quadratic band touching point enters QAH under weak repulsion.

Chern number by flux insertion

$$C = \frac{1}{2\pi}\int d\phi_x d\phi_y (\partial_{\phi_x}\langle\Omega(\phi_x,\phi_y)|\partial_{\phi_y}|\Omega(\phi_x,\phi_y)\rangle - \partial_{\phi_y}\langle\Omega(\phi_x,\phi_y)|\partial_{\phi_x}|\Omega(\phi_x,\phi_y)\rangle$$





The tower of states crosse with higher continuum at some flux, so that the calculation cannot proceed, maybe because the twisted boundary frustrates the current loops.

Twofold screw axis and inversion

Twofold rotation and inversion imply an at-center mirror plane

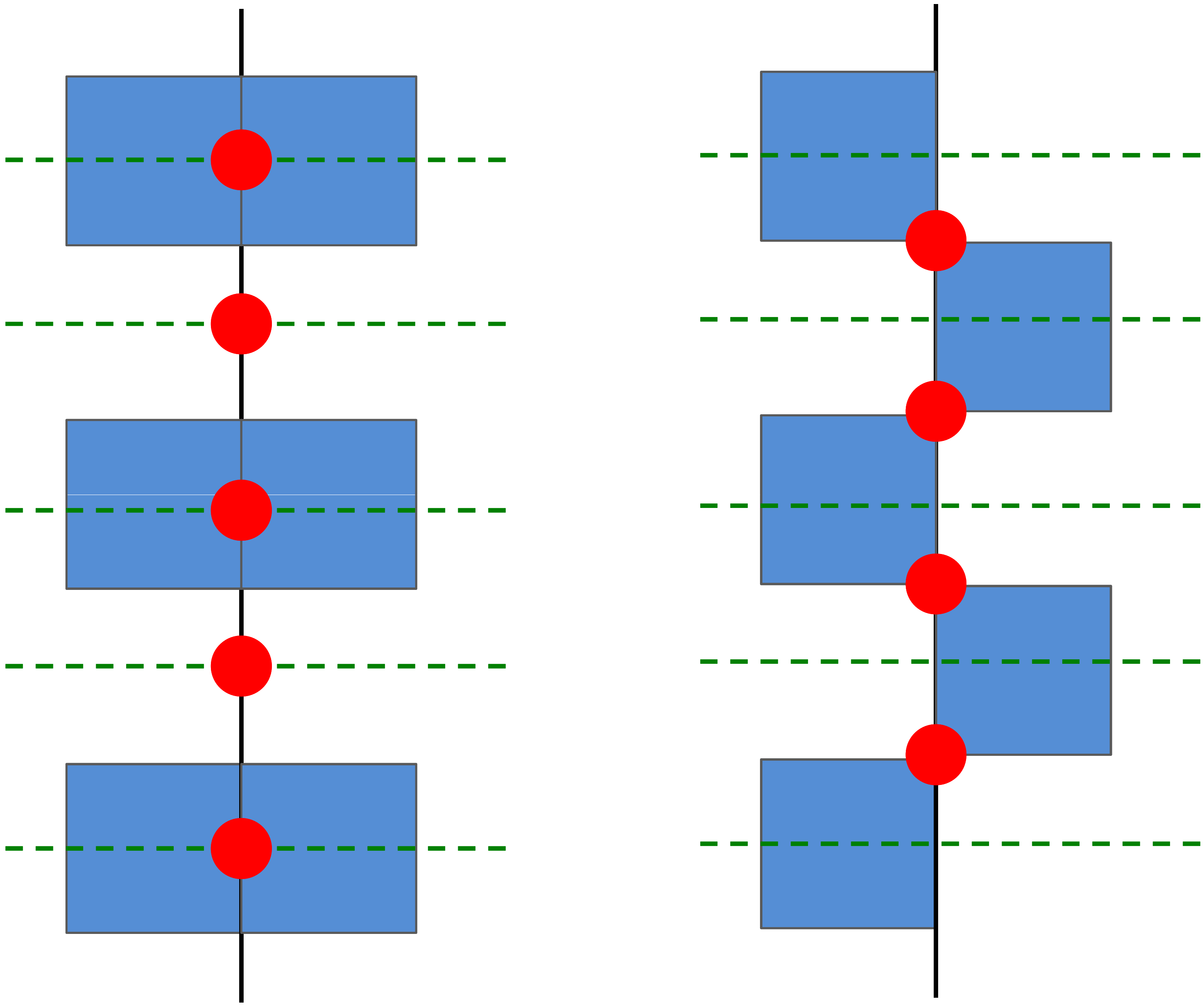
$$C_2 : (x, y, z) \to (-x, -y, z)$$

$$M \equiv C_2 * P : (x, y, z) \to (x, y, -z)$$

Twofold screw and inversion imply an off-center mirror plane

$$S_2 : (x, y, z) \to (-x, -y, z + 1/2)$$

$$M \equiv S_2 * P : (x, y, z) \to (x, y, -z + 1/2)$$



Off-center mirror plane

- An off-center M does not commute with P.

$$M * P = T_z * M * P = e^{-ik_z} M * P$$

- At kz=0, the degenerate pair have opposite mirror eigenvalues.

$$|\psi_2(\mathbf{k})\rangle = P * T|\psi_1(\mathbf{k})\rangle \quad M^2 = -1 \quad M|\psi_1\rangle = +i|\psi_1\rangle$$

$$M|\psi_2\rangle = MPT|\psi_1\rangle = PTM|\psi_1\rangle = PT(+i)|\psi_1\rangle = -iPT|\psi_1\rangle = -i|\psi_2\rangle$$

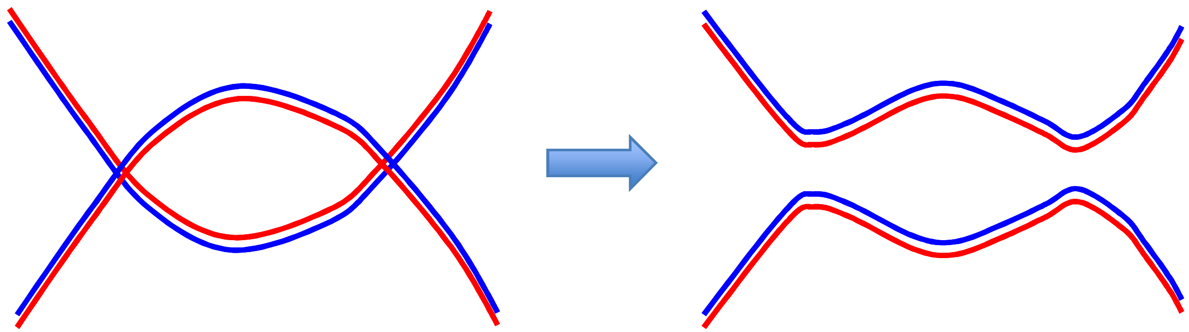
- At kz=pi, they have the same eigenvalues.

$$M|\psi_2\rangle = MPT|\psi_1\rangle = -PTM|\psi_1\rangle = -PT(+i)|\psi_1\rangle = +iPT|\psi_1\rangle = +i|\psi_2\rangle$$

CF*, Y. Chen, H.-Y. Kee and L. Fu, Phys. Rev. B 92, 081201(R) (2015)

Accidental vs robust nodal lines

- At kz=0, crossings are accidental



- At kz=pi, line crossings are robust